An Atmospheric Science Observing System Simulation Experiment (OSSE) Environment

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***Abstract*— An atmospheric sounding mission starts with a wide range of concept designs involving measurement technologies, observing platforms, and observation scenarios. Observing system simulation experiment (OSSE) is a technical approach to evaluate the relative merits of mission and instrument concepts. At Jet Propulsion Laboratory (JPL), the OSSE team has developed an OSSE environment that allows atmospheric scientists to systematically explore a wide range of mission and instrument concepts and formulate a science traceability matrix with a quantitative science impact analysis. The OSSE environment virtually creates a multi-platform atmospheric sounding testbed (MAST) by integrating atmospheric phenomena models, forward modeling methods, and inverse modeling methods. The MAST performs OSSEs in four loosely coupled processes, observation scenario exploration, measurement quality exploration, measurement quality evaluation, and science impact analysis.**

I. INTRODUCTION

NASA's Earth atmospheric science missions study the physical properties of Earth's atmosphere (such as pressure, temperature, wind, humidity, aerosols, and trace gases) by employing a wide range of atmospheric sounding systems. During the mission study phase, scientists specify science objectives of the mission and develop measurement requirements corresponding to the science objectives. The measurement requirements must be traceable by clearly establishing the relationship between the science objectives and the properties of platforms and instruments. Scientists express the relationship with a two dimensional array referred to as a science traceable matrix, where the x-axis represents the instrument properties and the platform properties and the y-axis represent the science objectives.

An emerging new paradigm in Earth science missions addresses the interplay between observing systems and Earth system models where observations are assimilated to validate the models and simulated experiments are performed to optimize future observations. The new paradigm provides a bridge between scientists and engineers allowing them to collaboratively explore many questions such as

- What needs to be measured?
- When and where?
- How often and how long?
- How accurately & how precisely?

To address the above questions systematically for future atmospheric science missions, the OSSE team at Jet Propulsion Laboratory (JPL) has developed an atmospheric sounding OSSE environment that can provide scientists a multi-platform atmospheric sounding test-bed (MAST). The MAST allows scientists to populate the science traceability matrix with a comprehensive science impact analysis by exploring a wide range of "what-if" scenarios. Scientists perform the what-if exploration in two levels, a mission level and an instrument level. The mission level explores when, where, and how often observations should be made while the instrument level explores how accurately and how precisely the samples should be measured as shown in Figure 1.

The major challenges in developing the MAST include parametric representation of the measurement requirements, rapid exploration of the requirement trade space, and quantitative merit evaluation of the requirements. Section 2 presents a formulation process where an observation scenario is composed as a list of targets to be sampled and the measurement quality is composed as a list of instrument performance parameters. Section 3 presents the forward modeling process that simulates measurements by modeling the target atmospheric phenomena and instrument performance as specified during the formulation process. Section 4 presents the inverse modeling process that estimates an atmospheric state variable from the simulated measurements and assimilates the estimated states for global forecasting. The retrieval and assimilation sensitivities of the explored parameters populate the science traceability matrix. Finally, Section 5 concludes the paper with a brief summary of the current status and the future direction of the atmospheric sounding OSSE environment research at JPL.

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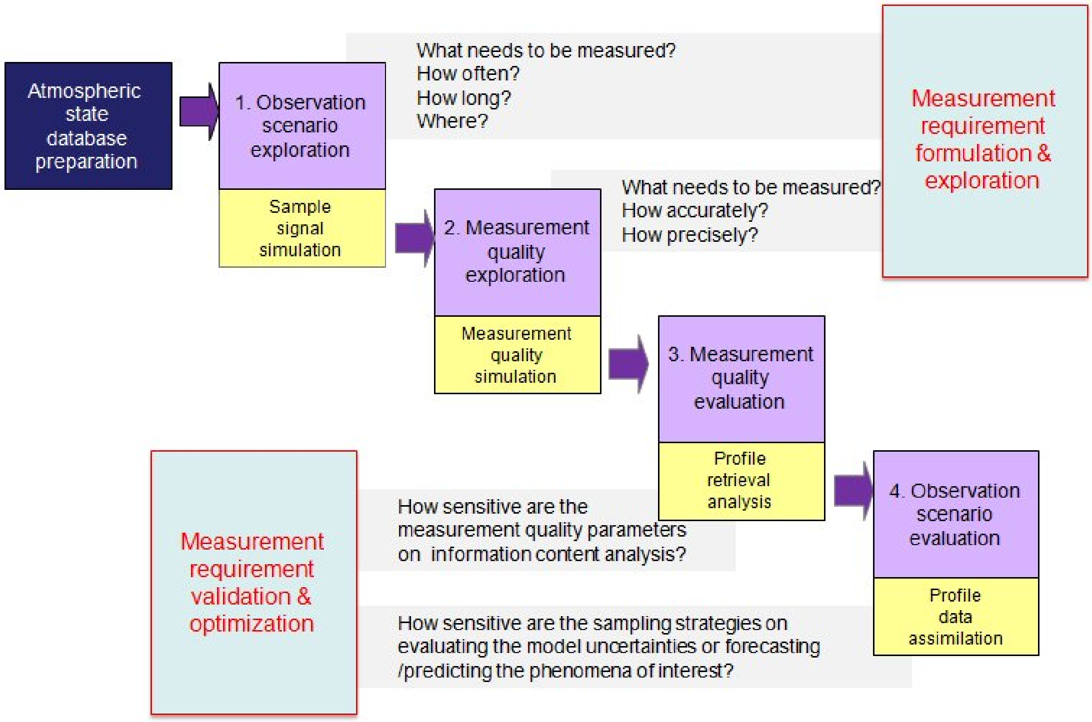

Figure 1. Four-stage OSSE process for traceable measurement-requirements formulation

II. FORMULATION PROCESS

The MAST represents the Earth system with a comprehensive atmospheric state database that can provide a proper representation of the observed phenomena. The preparation of a comprehensive atmospheric state database that allows sampling of the target atmospheric state variables in the observation scenario is a prerequisite for performing OSSEs. The atmospheric state variables include pressure, altitude, humidity, temperature, aerosols, land and ocean reflectance, and trace gases (e.g., ozone [O3], cartbon monoxide [CO], nitrogen oxides [NOx]). Multiple models are integrated to prepare a complete phenomena database. This includes Global Earth Observation System (GEOS) for meteorology data, GEOS-Chem for trace gases, International Multi-user Plasma Atmospheric and Cosmic Dust Twin laboratory (IMPACT) for aerosols, and Moderate Resolution Imaging Spectrometer (MODIS) for surface reflectance. Each state variable is filed daily and the content is ordered by time, vertical levels, latitudes, and longitudes for cross referencing among the state variables.

A set of mission design tools [1] allow scientists to compose mission and instrument concepts with low Earth orbiters and geo-stationary orbiters. The mission design tools translate the concepts into sample lists and instrument lists representing observation scenarios and measurement quality requirements. With the mission design tools, scientists can specify a mission concept by selecting an orbit type and specifying options temporal constraints (day, night, anytime), spatial selections (land, ocean, coast, anywhere), and sampling frequencies (sampling interval). The mission concept specification is translated into a list of samples where each sample is described with time, location, and platform position and orientation. Scientists can compose multiple observation scenarios by varying the orbit type or the options for sampling methods. For example, an observation scenario covering a day period of a geo-stationary orbit measuring 20 by 20 deg area in one-degree resolution every three hours would generate 2400 samples.

Scientists can also specify the measurement fidelity by setting the spectral coverage, number of channels, channel shape, signal to noise ratio (SNR) or noise equivalent spectral radiance (NESR) , and spectral linearity. Scientists can experiment a wide range of properties by simply setting the value range and increment for each quality parameter. An instrument property list is automatically populated with all possible combinations of the property values within the specified range. For example, when the scientists specify the SNR range from 100 to 500 with an increment of 100, and the nunmber of channel range from 100 to 1000 with an increment of 100, 50 property-variations (5 SNR variations combined with 10 channel variations) will populate the instrument list.

The sample lists and instrument lists represent the exploration space defined by scientists for performing the four-stage OSSE process [2]. The first stage explores the samples in the sample list by composing the atmospheric states and transforming them to signal radiance spectra. The second stage explores the instrument properties in the instrument list by applying corresponding distortions to the signal radiances and simulating the noise. The third stage evaluates the measurement quality by retrieving the profile of a desired state variable from the simulated measurements and statistically analyzing the retrieval performance sensitivity with respect to a specific instrument property parameter. The final stage evaluates observation scenarios by assimilating the retrieved profiles and analyzing the convergence behavior of the assimilated state to the reference atmospheric state over the entire observation period.

The OSSE website allows retrieval of the results at each stage for interactive viewing as well as file downloading. The explicit user control of the dataflow among the four stages is intended to allow a flexible combination of the observation scenarios and measurement qualities for exploring a wide range of mission and instrument concepts with the integrated evaluation of multiple measurement types for retrieval sensitivity and data assimilation accuracy. The exploration service also allows scientists to submit externally prepared atmospheric state profiles for performing special-purpose OSSEs. Figure 2 depicts the relationship between the design tools and on-line services.

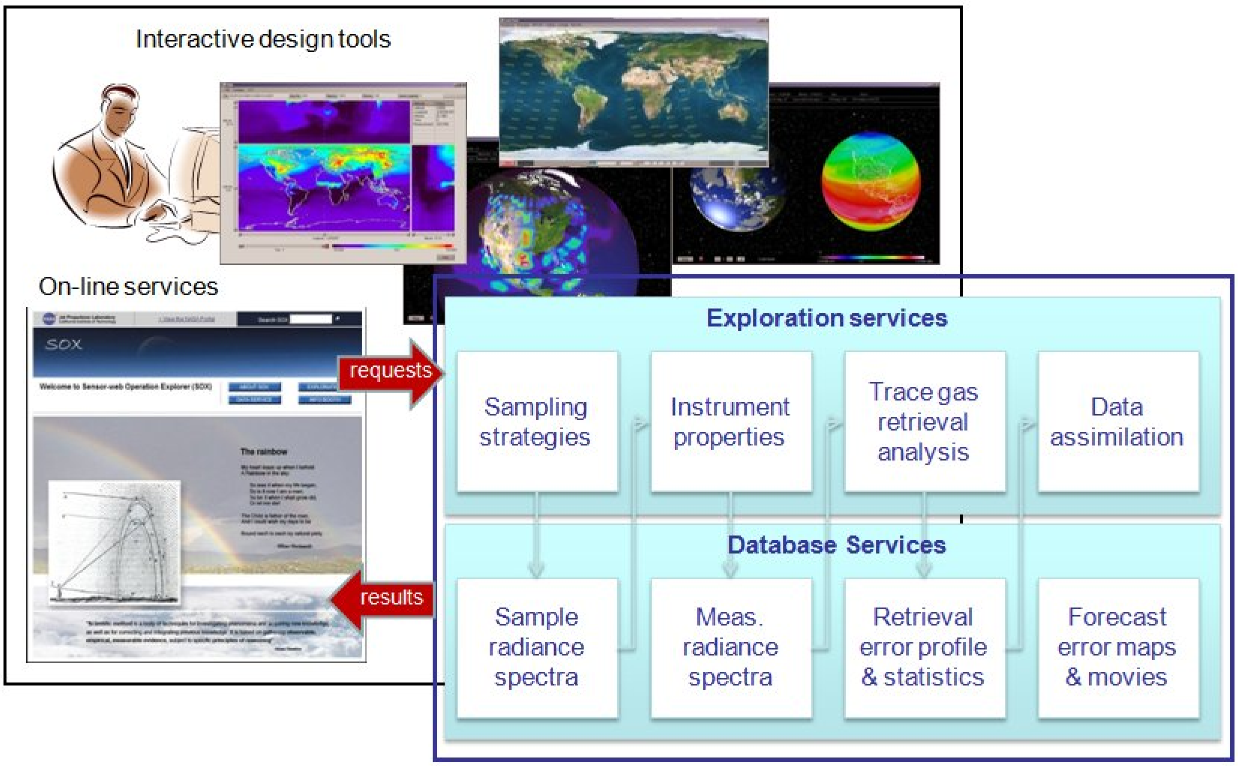

Figure 2. Exploration process with interactive design tools and on-line services

III. FORWARD MODELING

A forward model is an approximate representation of the measurement physics, which is constructed based on how the measuring device works and how the information is extracted from the measurements. The three major forward-modeling components are: 1) atmospheric state vector, 2) radiative transfer function; and 3) instrument performance. The atmospheric state vector defines the phenomena property of the atmospheric path, the radiative transfer function defines the monochromatic radiance emerging from an atmospheric path, and instrument performance defines signal detection sensitivity, distortion, and noise. Figure 3 illustrates an example of the forward modeling process.

For each sample, a state vector is composed by tracing the atmospheric path defined by the viewing geometry of the platform at the specified time and location. The atmospheric state vector is stored as a binary data file with an XML header that describes the dimensionality, phenomena type, phenomena component name, physical unit, and data type. The state vectors for the physical parameters and trace gases represent the altitudinal profile, while the optical depth and single-scattering albedo resulting from each aerosol type and the surface reflectance represent the spectral profile. The seasonal variation of the direct reflectance spectrum is modeled based on the data products of the MODIS instrument on the Terra satellite [3]. The ocean surface, the direct and diffused reflectance spectra are simulated with a parametric model that takes into account for wind speed and Chlorophyll density [4].

A radiative transfer model (RTM), transforms the state vector to a radiance spectrum by attenuating the solar irradiance spectrum with the integrated optical depths of the atmospheric path. The optical attenuation from each component in the state vector is sensitive to the frequency range. For example, the optical attenuation from the aerosols may be negligible over the infrared range but it is significant over the ultraviolet and visible range. In order to address the frequency dependency in a computationally effective manner, linearized discrete ordinate radiative transfer (LIDORT) is used for ultraviolet and visible range while line by line RTM (LBLRTM) is used for infrared range.

The RTMs are community-developed software with model-unique input and output format requirements. The RTM-independent atmospheric state representation allows the phenomena model database to be decoupled from the software implementation details of the RTMs [5]. The signal radiance spectrum has much higher (greater than 1000 times) spectral resolution than that of explored observing system in order to accurately simulate the spectral line shape and linearity properties.

The measurement simulation is performed in multiple steps, each step applying a specific instrument performance property. First, a bandpass filtering is applied to extract the specified spectral range from the input radiance spectrum. Second, a convolution kernel is formulated based on the line-shape and line-width specification. The convolution kernel is applied to the bandpass-filtered spectrum while observing the specified linearity variation. Third, after the convolved signal radiance is converted to photon counts, the SNR property is simulated by scaling the signal strength and adding the system noise. Finally, the noisy signal is quantized within the specified digital number range.

Figure 3 depicts the transformation flow of the atmospheric state to signal radiance spectrum and the signal-radiance spectrum to instrument measurements. The atmospheric state is illustrated with the altitudinal profiles of Ozone, temperature, and dust. The signal radiance spectrum covers the spectral range of 900 to 1200 wave numbers with the spectral resolution of 1.0e-3 wave number. The two measurement spectra represent the instrument response of two spectral resolutions, 0.1 and 1 wave number. The instrument simulator integrates an imager, a spectrometer, and a radiometer to model spatial, spectral, and intensity distortions of a signal by an instrument system.

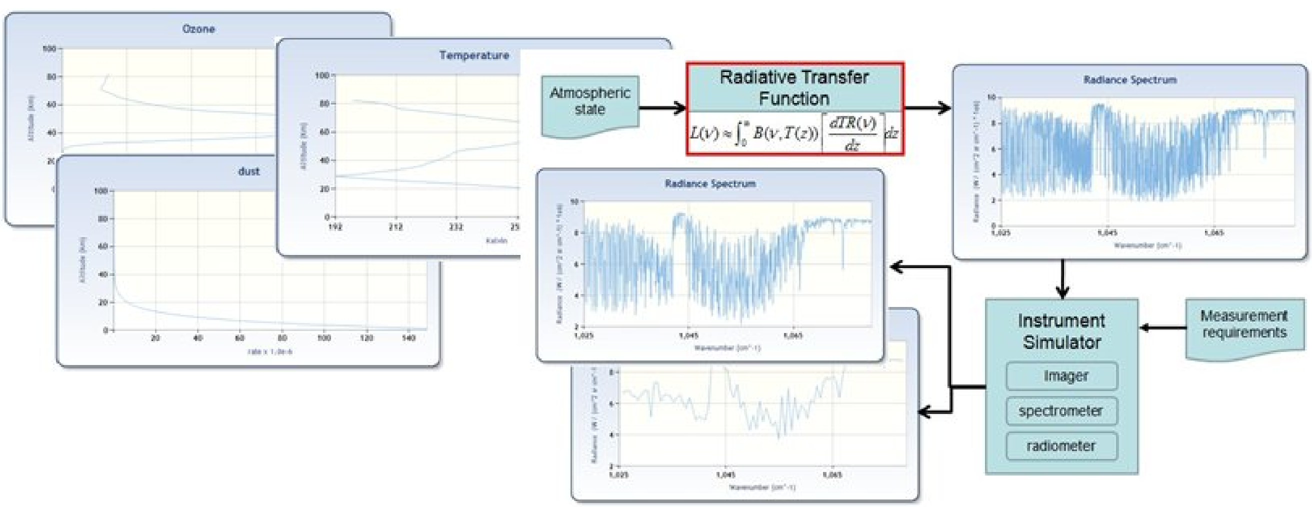

Figure 3. **Information transformation flow of the forward modeling process**

IV. INVERSE MODELING

The atmospheric sounding instrument measures electromagnetic radiation emerging from an atmosphere from which the distribution of constituents may be retrieved. When the measurements are indirectly made, the inversion of the forward modeling is required to retrieve the desired information. The retrieval analysis may be applied to any subset of the atmospheric state. The trace-gas density is estimated by applying the inverse averaging kernel to the measurement. The evaluation process involves the following three steps: 1) add simulated noise to the measurement and the Jacobean radiance; 2) perform a linear retrieval that computes the averaging kernel, retrieval gain, and vertical resolution; and 3) calculate the retrieval-error statistics and distribution with respect to the measurement requirement parameters explored [6]. The retrieval accuracy is used to formulate a statistical distribution of the sensitivity of the design parameters such as sampling frequency, spectral resolution, and SNR. The sensitivity analysis provides a quantified design impact on science return, thus allowing science-driven requirements formulation.

For global data assimilation, the MAST utilizes GEOS-Chem-Adjoint [7], a standardized adjoint of the GEOS-Chem. GEOS-Chem is a global 3D model of atmospheric composition driven by assimilated meteorological observations from the Goddard Earth Observing System (GEOS) of the NASA Global Modeling and Assimilation Office. The global data assimilation optimizes the combination of three sources of information: an a priori state, a forward model of physical and chemical processes, and observations of some state variables. The observations in this case refer to the retrieved vertical profile of the trace gas components, generally known as level-2 mission data products.

Adjoint models are powerful tools widely used in meteorology and oceanography for applications such as data assimilation, model tuning, sensitivity analysis, and determination of singular vectors. The GEOS-Chem-Adjoint provides adjoint models for chemistry, advection, convection, and deposition/emission. The adjoint model computes the gradient of a cost function with respect to control variables. Generation of adjoint code may be seen as the special case of differentiation of algorithms in reverse mode, where the dependent function is a scalar. Developing a complete adjoint of global atmospheric models involves rigorous work of constructing and testing adjoints of each of the complex science processes individually, and integrating those adjoints into a consistent adjoint model [8].

The mathematical formulation for calculating gradients of a model output using the adjoint method can be derived from the equations governing the forward model analytically or discretely. The adjoint sensitivity analysis approach is receptor-oriented, and it traces backward in time for the cause of a perturbation in an output variable contrast to the forward sensitivity analysis, which propagates the initial perturbation forward in time. The sensitivity mode allows collaborative observation planning between air-borne and space-borne missions as well as targeted observation planning [9].

The global data assimilation stage can be also applied to the real observation data to study the model uncertainties or retrieval uncertainties. Recently, the GEOS-Chem-Adjoint has been applied to microwave limb sounder (MLS) level-2 data products of ozone observation. Figure 4 illustrates a frame of the MLS ozone assimilation result where the four panels represent the global ozone distribution at 60 hPa on 4^{th} of July in 2006 for GeosChem model (upper left), MLS assimilated (lower left), MLS observation contribution ratio (upper right), and assimilation deviation ratio (lower right). The frame indicates that the MLS observation shows higher concentration of ozone at the North and South Polar regions and lower concentration at the Equator region than that of GEOS-Chem. The GEOS-Chem-Adjoint assimilates the observations in a four-hour interval and the upper right panel indicates the samples assimilated during that interval.

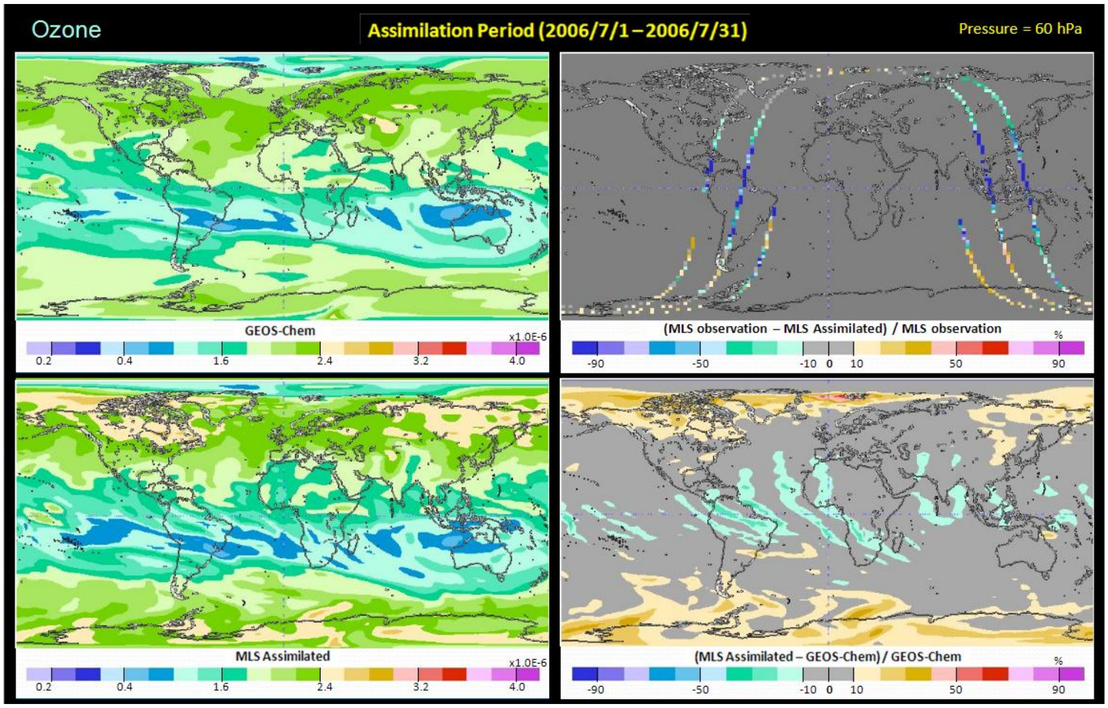

Figure 4. **GEOS-Chem-adjoint process for MLS ozone data assimilation**

V. CONCLUSION

The MAST provides an end-to-end OSSE process that can quantitatively evaluate the science impacts of instrument concepts and sampling strategies. The end-to-end OSSE process is organized in four stages; (1) observation scenario exploration, (2) measurement quality exploration, (3) measurement quality evaluation, and (4) observation scenario evaluation. An OSSE website provides JPL atmospheric scientists to perform OSSEs by interactively controlling the above four processes. The first two stages are referred to as forward modeling and the last two stages are referred to as inverse modeling. The forward modeling allows parametric formulation of the mission and instrument concepts and accurate simulation of resulting measurements while the inverse modeling provides quantitative evaluation of the science impact of the explored concepts with respect to retrieval analysis and global data assimilation.

The MAST is currently supporting GEOCAPE (Geostationary Coastal and Air Pollution Events) concept study (lead: Dr. Annmarie Eldering/JPL), part of Tier-2 missions recommended by the NRC decadal survey. The MAST is being utilized to evaluate the advantage of geostationary orbit over low-Earth orbit and to explore the detailed science return from improved measurement capabilities including spectral coverage (IR, UV, IR+UV), spectral resolution, and signal-to-noise ratio. The science impact evaluation is with respect to chemical data assimilation for improved air quality forecasts, pollutant emission monitoring, and regional-scale to intercontinental-scale pollution transport.

The MAST capabilities will be extended to support the CLARREO (Climate Absolute Radiance and Refractivity Observatory) concept study part of Tier-1 missions recommended by the NRC decadal survey, for mission design and virtual observation for climate model uncertainty evaluation. The largest source of uncertainty for climate prediction is climate feedbacks that are coupled radiative response of the hydrological cycle to anthropogenic forcing. The MAST will be employed to evaluate the sensitivity of the climate feedbacks which are manifested at unresolved scales for contemporary climate models and the proposed CLARREO footprint.

The future research areas of interest include a web-based model integration infrastructure that provides a dynamic coupling of global and regional phenomena models, a model-based system engineering process that comprehensively validates and verifies instrument design and mission planning, and a heterogeneous data assimilation method that can rapidly assimilate observations from multiple sensors on multiple platforms. The extended capabilities will support Global Climate and Environment (GC&E) program at JPL for designing a global emission monitoring system infrastructure.

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